Modeling of Graphene Membrane Rupture with Density Functional Tight Binding

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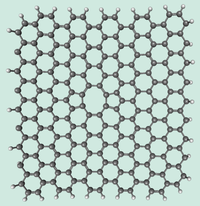
Abstract

Density Functional Tight Binding (DFTB) is being used to find the cause of the catastrophic rupture of a graphene membrane under the effect of an electric field. Efforts are also being made to increase the computational efficiency of the program by replacing LAPACK calls with ScaLAPACK calls.

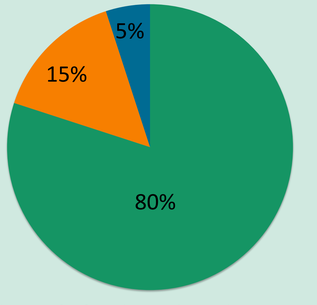


Introduction

DFTB+ is being used to find out why a graphene membrane is rupturing under an electric field. When an electric field of 3 V/nm is applied to a graphene membrane suspended in a 1 M KCl solution, the membrane ruptures catastrophically, sometimes ripping completely in half.

Carbons	Corners	Defect
218	Free	Mono-vacancy
		Di-vacancy
		Reconstructed di-vacancy
	Frozen	Mono-vacancy
		Di-vacancy
		Reconstructed di-vacancy
508	Free	Mono-vacancy
		Di-vacancy
		Reconstructed di-vacancy
	Frozen	Mono-vacancy
		Di-vacancy
		Reconstructed di-vacancy

Several different variations of graphene membranes are being tested under varying conditions using molecular dynamics (MD) simulations.



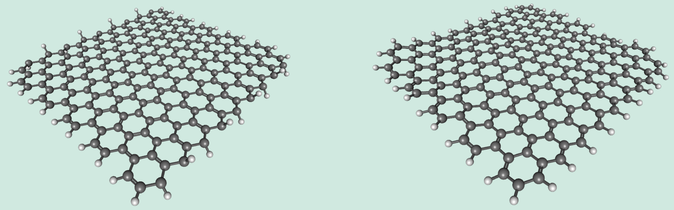
These can be seen in the above table. Simulations are run on Beacon using Intel's multi-threaded MKL.

The most computationally expensive component of DFTB code is its linear algebra operations.

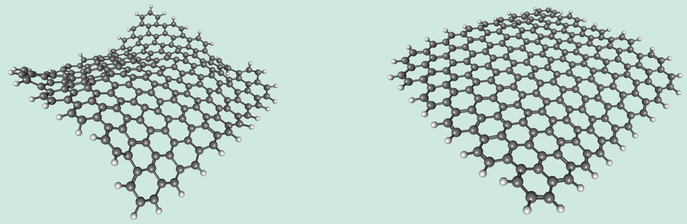
As conditions for the calculations become more complex the time also increases.

Simulations

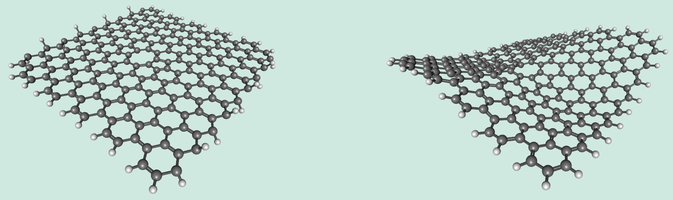
To simulate a 3 V/nm electric field in DFTB+, a 15 eV point charge is placed 100 Å away, along a vector normal to the membrane. A -15 eV point charge mirrors the first on the other side of the membrane. Below is the flat membrane before (left) and after (right) the MD simulation.



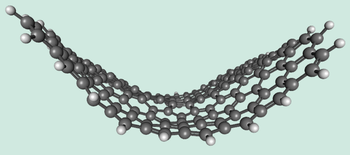
Below are the input and output geometries of a warped membrane.



Below are the input and output geometries of a defective membrane.

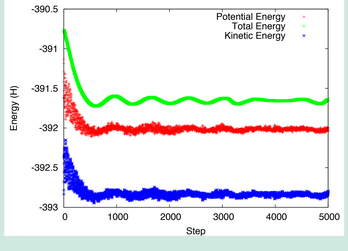


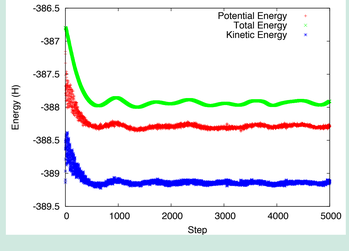
Ongoing simulations will attempt to force an ion through the membrane.



Simulations of the defective membrane exhibited more folding than pristine membranes.

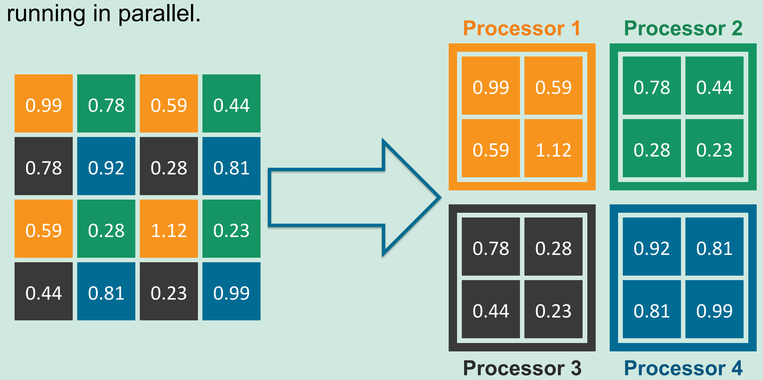
Changes in the membranes' energies were recorded during MD simulations. The energy plots of the flat (left) and defective membranes (right) were virtually identical.





LAPACK to ScaLAPACK

Current DFTB code utilizes LAPACK (Linear Algebra Package) function calls to perform its linear algebra operations such as matrix-matrix multiplication, Cholesky factorization, and diagonalization. By replacing the LAPACK routines with ScaLAPACK (Scalable LAPACK) routines, the calculation speed can be improved. ScaLAPACK has the advantage of distributing the matrix data in a block-cyclic fashion to processors running in parallel.



A comparison of operations on a 16834 X 16834 matrix showed ScaLAPACK calls were faster. Their efficiency can be further improved by increasing the number of processes and threads.

LAPACK	Time (s)	ScaLAPACK	16 Processes Time (s)	25 Processes Time (s)	36 Processes Time (s)
DGEMM	40.0	PDGEMM	38.2	23.5	18.3
DPOTRF	6.7	PDPOTRF	7.4	5.0	3.6
DPOTRI	25.1	PDPOTRI	23.0	21.1	16.8
DSYEV	365.2	PDSYEV	259.2	190.4	151.2
DSYEVD	254.6*	PDSYEVD	215.5	89.6	71.2
DSYGVD	333.1	PDSYGVX	185.6	136.5	105.9

All calculations performed on Beacon, except those marked with *, which were performed on Darter

Acknowledgements

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References

Colapinto, J. Material Question. *The New Yorker*, 2014
Daniels, C.: Horning, A.; Phillips, A.; Massote, D.; Liang, L.; Bullard, Z.: Sumpter, B.; Meunier, V. Mechanisms of Stress Release in Graphene Materials.
Koskinen, P.; Mäkinen, V. Density-Functional Tight-Binding for Beginners. *Computational Materials Science.* 2009, *47*, 237-253.
DFTB+[Computer software].(2013).Retrieve from http://www.dftb-plus.info
NETLIB Repository. University of Tennessee-Knoxville & Oack Ridge National Lab. Web. 7 Jul. 2015